

Fluopropanate-sodium
22898-01-7 | DTXSID9066837

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: $2.99\text{e-}13 \text{ cm}^3/\text{molecule}\cdot\text{sec}$

Global applicability domain: Inside

Local applicability domain index: $3.23\text{e-}01$

Confidence level: $5.71\text{e-}01$

Nearest Neighbors from the Training Set

Image not found

Acetic acid, trifluoro-

Measured: $1.20\text{e-}13$

Predicted: $1.81\text{e-}13$

Image not found

Acetic acid, trifluoro-, methyl ester

Measured: $5.20\text{e-}14$

Predicted: $5.42\text{e-}14$

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1,1,2,3,3,3-Hexafluoro-1-propene

Measured: $2.20\text{e-}12$

Predicted: $2.03\text{e-}12$

Image not found

Hexafluorobenzene

Measured: $1.71\text{e-}13$

Predicted: $6.65\text{e-}14$

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Ethene, 1,1-dichloro-2,2-difluoro-

Measured: $7.35\text{e-}12$

Predicted: $5.42\text{e-}12$